Controlling the Biological Effects of Spermine Using a Synthetic Receptor

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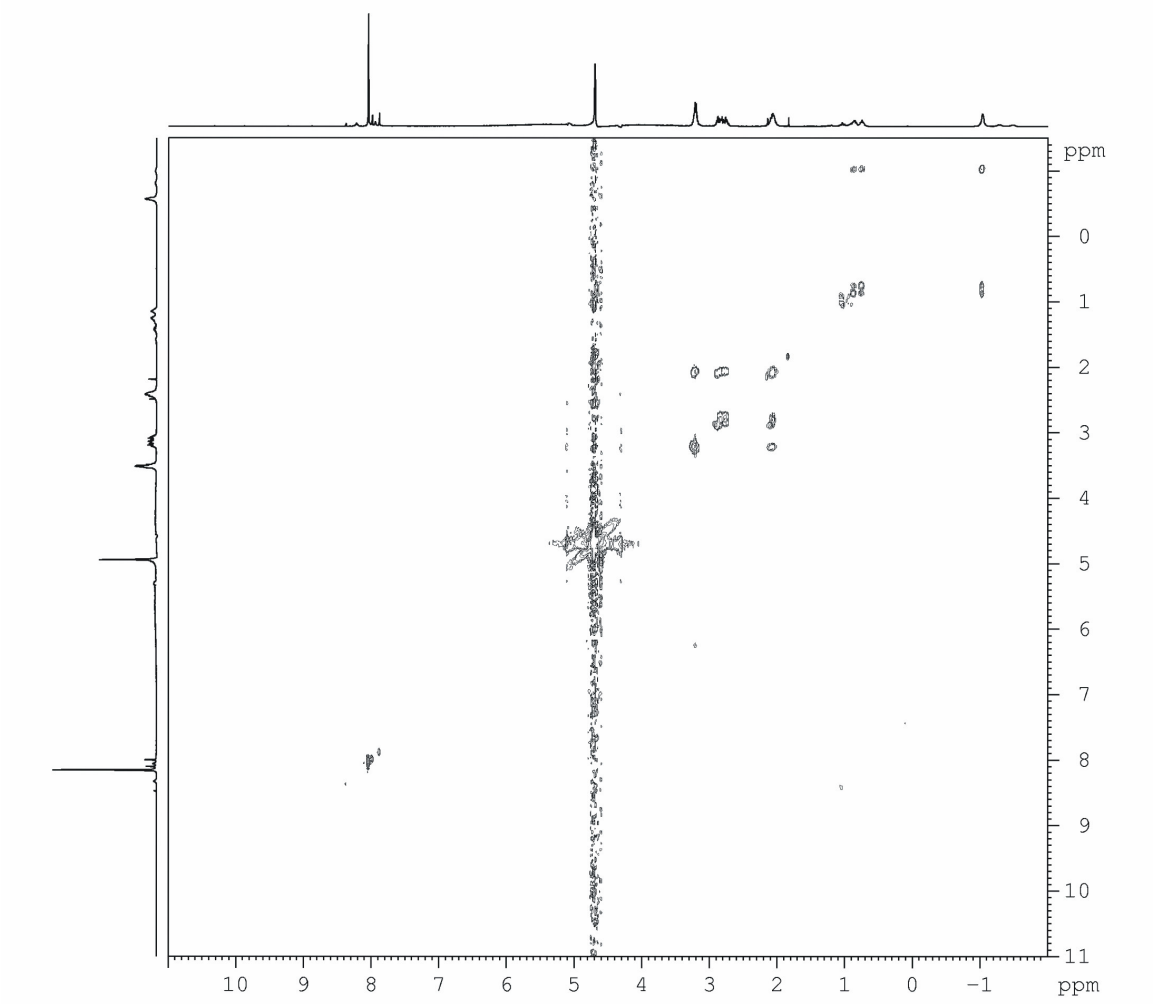

Figure S1. COSY spectrum of the complex between spermine and **6**. Solvent: 89 mM phosphate buffer (pH 7.4, 11% D2O)

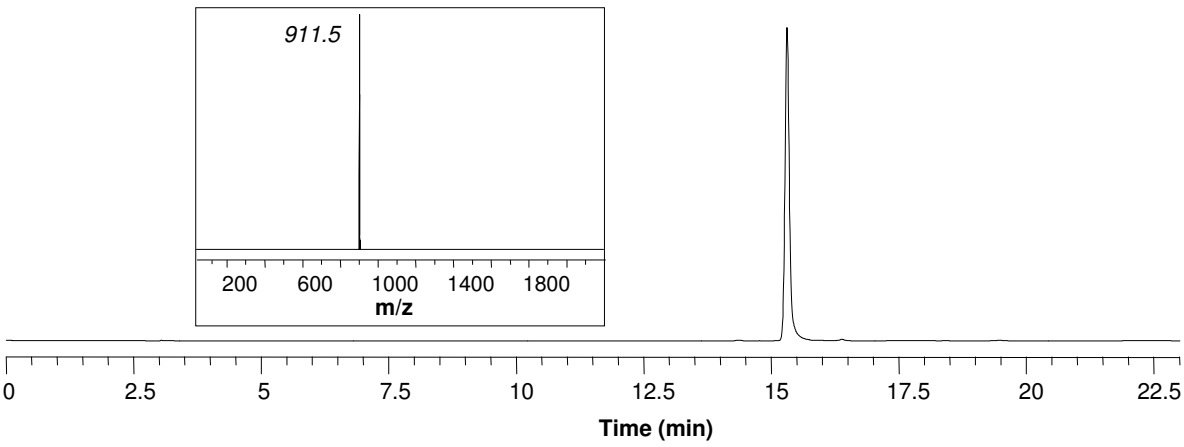

Figure S2. HPLC and MS (inset) analysis of **6**.

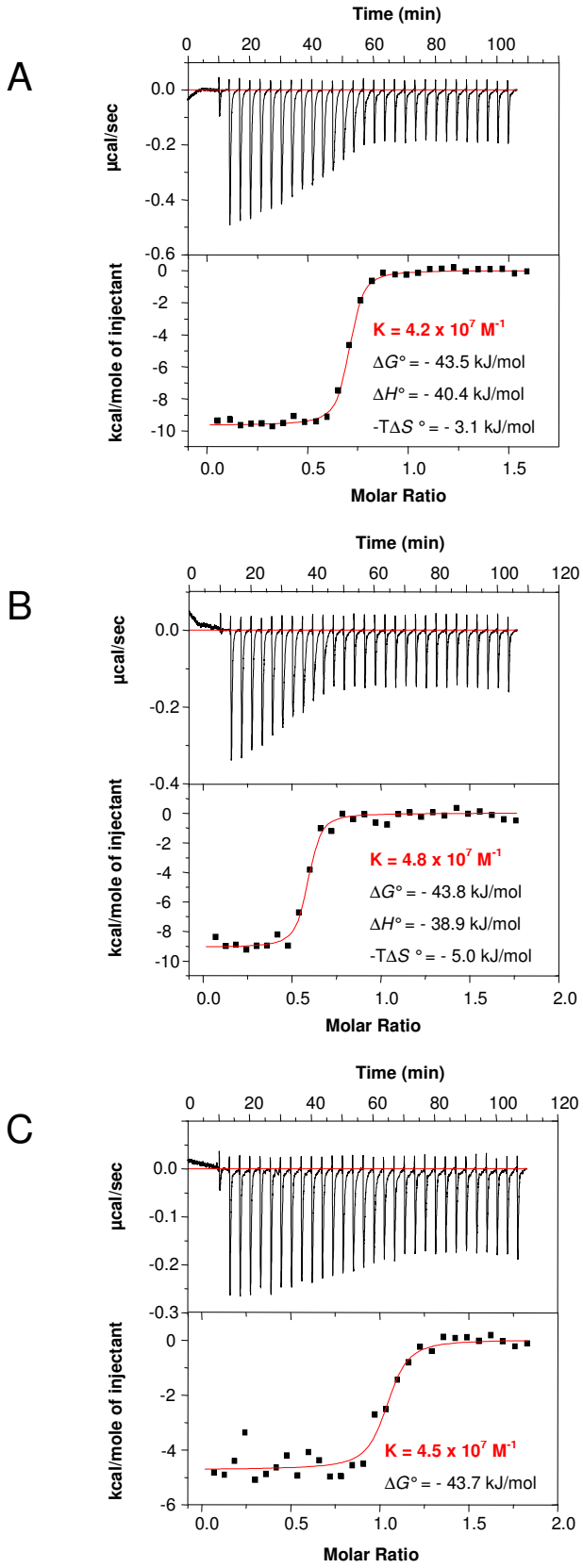

Figure S3. ITC data. Concentrations of **1** and **6** are 0.1068 mM and 0.0156 mM (A), 0.0739 mM and 0.0098 mM (B), 0.0528 mM and 0.0070 mM (C) respectively.

Table S1. Energies of the free receptors and complexes as determined by molecular dynamics simulations.

Species	***Relative configurations of the disulfide bonds***	***MD Energies Average Total Energy*** *(kJmol^{-1})*	***Relative MD Energies***[(a)] *(kJmol^{-1})*
Receptor	(*P*,*P*,*P*,*P*)	-1785.89	5.83
	(*P*,*P*,*P*,*M*)	-1786.73	4.99
	(*P*,*P*,*M*,*M*)	-1784.50	7.22
	(*P*,*M*,*P*,*M*)	-1791.72	0
Complex	(*P*,*P*,*P*,*P*)	-2735.61	0
	(*P*,*P*,*P*,*M*)	-2718.94	16.67
	(*P*,*P*,*M*,*M*)	-2715.36	20.25
	(*P*,*M*,*P*,*M*)	-2693.90	41.71

(a) MD energy relative to the most stable stereoisomer.